ON ATTRACTORS FOR A SHARP INTERFACE MODEL OF EXOTHERMIC PHASE TRANSITIONS

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Abstract

We study a free interface problem related to combustion of condensed matter and some non-equilibrium exothermal phase transitions. In spite of a variety of non-trivial dynamical scenarios exhibited by the model the solutions are uniformly bounded and the interface velocity is a smooth function. The main result of the paper establishes existence of a compact connected attractor for the classical solutions of the problem. Numerical evidence leads to the conjecture that the fractal dimension of the attractor is finite.

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1 Introduction

This paper presents a study of attractors for a two-phase Stefan problem with kinetics. We show that classical solutions of the problem approach a compact connected attractor in the uniform norm. We also demonstrate via direct numerical simulations that the attractor has a finite correlation dimension.

The free-boundary problem that is the subject of the paper arises naturally as a mathematical model of a variety of exothermic phase transition type processes, such as solid combustion [19] also known as Self-propagating High-temperature Synthesis or SHS [20], solidification with undercooling [17], laser induced evaporation [14], rapid crystallization in thin films [24] etc. These processes are characterized by production of heat at the interface, and their dynamics is determined by the feedback mechanism between the heat release due to the kinetics and the heat dissipation by the medium. In addition to its theoretical interest SHS has industrial applications as a method of synthesizing certain technologically advanced materials for high-temperature semiconductors, nuclear safety devices, fuel cells etc., see [20], [25] and also [26] for a popular exposition. SHS propagates through mixtures of fine elemental reactant powders (e.g., Ti + C, Ti +2B), resulting in the synthesis of compounds.

There is a substantial literature that treats analytical aspects of the initial–boundary value problem for different sharp-interface models with kinetics related to the problem (2.1-2.4) below, see [18, 27, 21, 3, 28, 5]. These works are concerned with basic issues of mostly local in time existence. See also [15, 29] where a *finite interval* version of the problem with linear kinetics and the asymptotic behavior when a kinetic parameter tends to zero are discussed. Dynamics on an semi-infinite spatial interrval for a one-phase model are investigated in [4]. The principal result of this paper is asymptotics for the position of the front $s(t)$ of the form $s(t) \sim kt^{\alpha} + O(t^{\beta})$ for $t \to \infty$, $0 < \beta < \alpha$, where $\alpha = 1/2$ or 1, depending on the value of undercooling. Needless to say that these asymptotics, being important on their own right, cannot capture order one variations in the temperature profile and velocity. These variations, their compact structure and presumably low Hausdorff dimension are the subject of our work (the graph of the time history of solutions in Fig. 1 below gives some idea about their complexity). We also note recent papers by Brauner *et al.,* [1]-[2], which study dynamical behavior of solutions of a related problem. In particular they consider perturbations of traveling-wave initial data and investigate their instability and bifurcations.

The objective of our work is to investigate asymptotic behavior of a propagating front. A variety of complex asymptotic dynamics (cf. [7]) arise only in the context of a infinite spatial interval. This necessarily calls for a problem on an *infinite* spatial domain, note that for a bounded domain the flame front reaches the external boundary in finite time and extinguishes. It is important to realize that the image of a ball under the evolution is not compact for any finite time. The potential theory computations in Sec. 3-4 allow us to extract the part of the evolution that compactifies (the contribution from the free interface), while the heat losses force the contribution from the initial conditions decay with time exponentially. We believe that this clear structure of the attractor indicates that careful potential theory estimates are unavoidable if one is to study asymptotic patterns and prove existence of a compact attractor in our case.

This study is partially motivated by numerical simulations and in particular by the numerical experiments described in [7], where it was demonstrated that the system generates a remarkable variety of complex thermokinetic oscillations. The dynamical patterns exhibited by the system, as the governing parameters are varied, include a Hopf bifurcation (see the rigorous proof [22]), period doubling cascades leading to chaotic pulsations, a Shilnikov-Hopf bifurcation etc. These patterns are well-known for the finite-dimensional dynamical systems and hint at the possibility that the essential dynamics of the free-interface problem may be finite-dimensional as well.

At the same time, in [8] we demonstrated that a 3×3 system of ODEs obtained as a pseudo-spectral approximation to the *one-phase* free-boundary problem exhibits dynamics that mimics that of the infinite-dimensional system to a surprising degree. For the one-phase problem we were able to prove that compactness and finite dimensionality of the attractor do take place [11].

It should be noted that the *two-phase* problem is somewhat more physically sound than its one-phase counterpart and appears in various applications. However, the methods of

the papers dealing with the one-phase problem are not directly applicable to the two-phase Stefan problem with kinetics which is the subject of the present communication. This is due to the additional temperature field behind the propagating interface (in the product phase) being not easily controllable. We overcome this difficulty in the present paper and show that the temperature behind the interface is sufficiently well-behaved to render compactness of the attractor.

Having proved compactness one is naturally curious as to how "large" is the attractor in terms of some appropriate measure. Currently we are not able to answer this question analytically due to, as we believe, purely technical difficulties although we have little doubt that the dimension is finite for the two-phase case. As the measure of complexity of the attractor and therefore of the asymptotic regime, we use the correlation dimension introduced by Grassberger and Procaccia (see, for example, [16]). The correlation dimension is based on the idea that if the evolution can be described by a finite number of degrees of freedom then the time series of observations on the system should be spatially correlated. This spatial correlation is measured by the corellation sum, which is directly related to the integral of the standard pair correlation function $c(\mathbf{r})$:

$$C(l) = \int_{|\mathbf{r}|\leq l} c(\mathbf{r}) d\mathbf{r}$$

If the dimension is ν then it is easy to see that $C(l) \sim l^{\nu}$ for small l. We compute the correlation dimension of the attractors generated in the direct numerical simulation of the problem.

The rest of the paper is organized as follows. In Sec. 2 we state the free-boundary problem and present some minimal background information on local existence and uniqueness. Sec. 3 and 4 constitute an analytical core of the paper. Here we employ the single-layer representation for the solution to obtain a natural decomposition of the solution into two contributions, one from the initial conditions, and another one from the free boundary. We obtain certain potential theory based estimates for both contributions to the solution and its spatial derivative, which are instrumental for the proof of compactness in Sec. 5. The estimates are proved to be uniform with respect to the sup norm of initial data, assuming that the nonlinearity in the kinetic free-boundary condition satisfies some natural requirements.

In Sec. 5 we utilize the estimates that show that the contributions from the free boundary are uniformly bounded and decay at infinity. Together with the uniform bound on the spatial derivative, they allow us to apply a version of the Arzela-Ascoli theorem, which guarantees that the contributions from the free boundary for initial data from a fixed ball form a precompact set. We complete the proof of existence of a compact attractor by using an appropriate abstract result from dynamical systems. Finally in Sec. 6, from direct numerical simulations of the free-interface problem we estimate the correlation dimension of the attractor.

2 The free-boundary problem. Local existence and uniqueness.

We study the following free boundary problem: find $s(t)$ and $u(x,t)$ such that

$$u_t = u_{xx} - \gamma u, \quad x \neq s(t) \tag{2.1}$$

$$u(x,0) = u_0(x) \geq 0 \tag{2.2}$$

$$g[u(s(t),t)] = v(t) \quad \text{for}\, t > 0, \tag{2.3}$$

$$[u_x(s(t),t)] := u_x^+(s(t),t) - u_x^-(s(t),t) = v(t) \quad \text{for } \ t > 0, \tag{2.4}$$

where $v(t)$ is the interface velocity, $s(t) = \int_0^t v(\tau)d\tau$ is its position, u is the temperature, and the derivatives u_x^+ and u_x^- are taken from right side and left side of the free interface respectively. The last term in the heat equation (2.1) is due to the heat losses into the medium surrounding the combustible or solidifying substance via Newton's cooling law with a non-dimensional coefficient $\gamma \geq 0$.

The surrounding matter is assumed to be at the temperature of the fresh combustible mixture at $-\infty$ (the original phase in the phase transition interpretation). By the same token the heat loss will reduce the temperature in the product phase to that of the medium. Thus the behavior of the solution at infinity should satisfy $\lim_{x\to\pm\infty} u(x,t) = 0$. It should be remarked that the presence of the heat losses $\gamma > 0$ only improves the analytical properties of the solutions. For $\gamma = 0$ the boundary condition at ∞ should be replaced by convergence to a constant.

The dynamics of the physical system are determined by the feedback mechanism between the heat release due to the kinetics $g(u|_{x=s(t)})$ and the heat dissipation by the medium. To illustrate the meaning of the kinetic term, for example, in the context of solidification, we note that for some substances in the presence of strong supercooling of the original phase the phase transition temperature measured at the interface may deviate considerably from the equilibrium one and is functionally related to the interface velocity. This dependence called the interface attachment kinetics can be different for different substances due to various microscopic mechanisms responsible for the incorporation of the product at the interface into the crystalline lattice.

The second interface condition (2.4) (the Stefan boundary condition) expresses the balance between the heat produced at the free boundary and its diffusion by the adjacent medium. As the problem describes propagation of the phase transition front, the first interface condition (2.3) is a manifestation of the *nonequilibrium* nature of the transition; its analog for the classical Stefan problem is just $u|_{x=s(t)} = 0$. We should mention that in contrast with the nonequilibrium problem, the dynamics of the classical Stefan problem is relatively trivial.

To discuss properties of the attracting set for classical solutions of the free interface problem (2.1)-(2.4) we need to first establish their existence and uniqueness for all times. We say that $u(x,t), v(t)$ form a *classical solution* of (2.1)-(2.4) if

(i) $u(x,t)$ and $v(t)$ are continuous for $t \geq 0$;

(ii) u_{xx} and u_t are continuous for $x \neq s(t),\ t > 0$;

(iii) Equations (2.1)-(2.4) are satisfied.

We quote the result as it was stated in [6]:

Theorem 1 *Suppose that the kinetic functions g satisfies the following assumptions:*
(A1) $g(u)$ is a continuously differentiable, monotone decreasing, negative function on $(0,\infty)$ with $g(0) = -v_0$ for some velocity $-v_0 < 0$;
(A2) $g(u)$ is sublinear: $\lim_{u\to\infty} g(u)/u = 0$;
and that the initial data $u_0(x) \geq 0$ are bounded.
Then there exists one and only one classical solution $u(x,t) > 0$ and $v(t)$ of the free interface problem (2.1)-(2.4). The solution is uniformly bounded for all $t > 0$.

For the reader's convenience we outline the scheme of the proof. First, the problem is reduced to an integral equation for the interface velocity using the single layer potential representation:

$$u(x,t) = e^{-\gamma t}\int_{-\infty}^{\infty} G(x,t,\xi,0)u_0(\xi)d\xi - \int_0^t G(x,t,s(\tau),\tau)e^{-\gamma(t-\tau)}v(\tau)d\tau, \tag{2.5}$$

where

$$G(x,t,\xi,\tau) = \exp\{-\frac{(x-\xi)^2}{4(t-\tau)}\}[4\pi(t-\tau)]^{-1/2} \tag{2.6}$$

is the heat kernel and $s(t) = \int_0^t v(\tau)d\tau$.

Taking the limit of (2.5) as $x \to s(t)$ and using the kinetics condition (2.3), we obtain an integral equation in terms of v only:

$$g^{-1}(v(t)) = e^{-\gamma t}\int_{-\infty}^{\infty} G(s(t),t,\xi,0)u_0(\xi)d\xi - \int_0^t G(s(t),t,s(\tau),\tau)e^{-\gamma(t-\tau)}v(\tau)d\tau, \tag{2.7}$$

Next, we show that for sufficiently small time intervals, the mapping K defined by the right hand side of the integral equation

$$v(t) = g\left[e^{-\gamma t}\int_{-\infty}^{\infty} G(s(t),t,\xi,0)u_0(\xi)d\xi - \int_0^t G(s(t),t,s(\tau),\tau)e^{-\gamma(t-\tau)}v(\tau)d\tau\right] := Kv \tag{2.8}$$

defines a contraction on an appropriately chosen closed set of continuous functions which yields local existence. We also remark that the velocity $v(t)$ can be shown to be an infinitely differentiable function. The centerpiece of the global existence proof is the *a priori* estimate, which allows us to extend the local solution indefinitely.

3 A priori estimates: spatial decay of solutions

In order to demonstrate existence of an absorbing set we need to establish spatial decay of the interface contribution to the classical solutions of the problem. First we obtain an estimate for the solution on the interface.

Theorem 2 *Let $u(x,t), v(t)$ be a classical solution of (2.1)-(2.4) and $||u_0|| = \sup_{-\infty<x<\infty}|u_0(x)| \leq M$, then*

$$|u(s(t),t)| \leq 2M + R_g, \qquad |v(t)| \leq g(2M + R_g) \tag{3.9}$$

where R_g and Λ are constants dependent solely on the kinetic function g.

Proof. First we prove the estimate for the interface temperature: $\psi(t) = g(v(t)) = I_1 - I_2$, where I_1 and I_2 are the two parts of the right hand side of (2.7).

It is rather obvious that $|I_1| \leq Me^{-\gamma t}$:

$$|e^{-\gamma t}\int_{-\infty}^{\infty} G(s(t),t,\xi,0)u_0(\xi)d\xi| = \frac{e^{-\gamma t}}{2\sqrt{t\pi}}||u_0||\int_{-\infty}^{\infty}\exp\{-\frac{(s(t)-\xi)^2}{4t}\}d\xi = e^{-\gamma t}||u_0||$$

Now, since the kinetic function satisfies the condition (A2), for any $\varepsilon > 0$ there exists $v_1 > 0$ such that $|g(\psi)/\psi| \leq \varepsilon$ if $g(\psi) \leq -v_1$. We subdivide I_2 as follows:

$$I_2 = \int_0^t G(s(t),t,s(\tau),\tau)e^{-\gamma(t-\tau)}g(\psi(\tau))d\tau = \int_{\chi_1} + \int_{\chi_2} = I_3 + I_4, \tag{3.10}$$

where $\chi_1 = \{\tau | -v_1 < g(\psi(\tau)) < -v_0, 0 < \tau < t\}$ and $\chi_2 = (0,t) \setminus \chi_1$.

For I_3 we have:

$$\begin{aligned}
|\int_{\chi_1} G(s(t),t,s(\tau),\tau)g(\psi(\tau))d\tau| &\leq v_1|\int_0^t G(s(t),t,s(\tau),\tau)d\tau| \\
&= v_1|\int_0^t \exp\{-\frac{(s(t)-s(\tau))^2}{4(t-\tau)}\}(2\sqrt{\pi(t-\tau)})^{-1}d\tau| \\
&\leq v_1|\int_0^\infty -\frac{2}{v_0\sqrt{\pi}}\exp\{-v_0^2\frac{t-\tau}{4}\}d(\frac{v_0\sqrt{t-\tau}}{2})| = \frac{v_1}{v_0}.
\end{aligned}$$

Here we have used the observation that $|s(t) - s(\tau)| = |v(\xi)|(t-\tau) \geq v_0(t-\tau)$ for some $\tau \leq \xi \leq t$.

Now, let us interpret $I_4(t) = P\psi(t)$ as a mapping; then the following estimate holds for its norm:

$$\begin{aligned}
\|P\psi\| &\leq |\int_{\chi_2} G(s(t),t,s(\tau),\tau)g(\psi(\tau))d\tau| \\
&\leq |\int_{\chi_2} G(s(t),t,s(\tau),\tau)\varepsilon\psi(\tau)d\tau| \\
&\leq \varepsilon\|\psi\|\,|\int_0^\infty G(s(t),t,s(\tau),\tau)d\tau| \leq \frac{\varepsilon}{v_0}\|\psi\|. \qquad (3.11)
\end{aligned}$$

Since $\psi = I_1 - I_3 - P\psi$, we have $\|\psi + P\psi\| = ||I_1(t) - I_3(t)|| \le M + v_1/v_0$. On the other hand, by choosing $\varepsilon = v_0/2$, we have $\|P\| \le \frac{1}{2}$, and therefore

$$|\psi(t)| = u(s(t), t) \le 2M + 2v_1/v_0.$$

The constant

$$R_g := 2v_1/v_0 \tag{3.12}$$

is the constant referred to in the statement of the theorem. Simultaneously,

$$|v(t)| \le g(2M + R_g) \tag{3.13}$$

■

Now using the uniform bounds for the interface velocity and temperature that we have just established it is easy to obtain the uniform estimate for the entire field through the maximum principle:

$$|u(x,t)| \le 2M + R_g, \tag{3.14}$$

From now on we shall assume that $g(u)$ is a monotonically decreasing differentiable function on $[0, \infty]$ with $|g'| \le C$ (recall that the velocity $v = g(u)$ is negative) and

$$v_0 \le -g(u) \le V_0 \text{ for some } V_0, v_0 > 0. \tag{3.15}$$

Both conditions are satisfied for the standard Arrhenius kinetics that in appropriate rescaled and normalized variables has the form (6.3). The existence of the lower bound v_0 in particular seems to be crucial for the uniform boundedness of solutions.

For the compacness result we need certain decay estimates for the contribution from the free boundary (see (3.17)-(3.18) below) which are established in the the following

Lemma 3 *Let $u(x,t), v(t)$ be a classical solution of (2.1)-(2.4) with $||u_0|| \le M$ then for the contribution from the free interface*

$$\Psi(x,t) = \int_0^t G(x, s(\tau), t-\tau) e^{-\gamma(t-\tau)} v(\tau) d\tau$$

the following estimates hold:
(i)

$$|\Psi(x,t)| \le \frac{V_0}{2\sqrt{\gamma}} \tag{3.16}$$

(ii) For $x < s(t)$

$$|\Psi(x,t)| \le \frac{V_0}{\sqrt{v_0^2 + 4\gamma}} \exp\{-\frac{v_0|x - s(t)|}{2} - \frac{|x - s(t)|^2}{4t}\} \tag{3.17}$$

(iii) For $x > s(t)$

$$|\Psi(x,t)| \leq \begin{cases} \dfrac{V_0}{\sqrt{\gamma}} \exp(-\alpha(x-s(t)), & \textit{for } x - s(t) > 2V_0/\gamma \\ \dfrac{V_0}{\sqrt{\gamma}}, & \textit{for } 0 < x - s(t) < 2V_0/\gamma \end{cases} \tag{3.18}$$

where $\alpha = \min(v_0/4, \gamma/2V_0)$.

Proof. First we obtain a very simple bound, which is valid for any x, t:

$$\begin{aligned} & |\int_0^t e^{-\gamma(t-\tau)} \frac{e^{-(x-s(\tau))^2/4(t-\tau)}}{\sqrt{4\pi(t-\tau)}} v(\tau) d\tau| \\ \leq & \; V_0 \int_0^t e^{-\gamma(t-\tau)} \frac{e^{-(x-s(\tau))^2/4(t-\tau)}}{\sqrt{4\pi(t-\tau)}} d\tau \leq V_0 \int_0^\infty e^{-\gamma s} \frac{ds}{\sqrt{4\pi s}} = \frac{V_0}{2\sqrt{\gamma}} \end{aligned}$$

Note that this estimate is very different from the one obtained through the maximun principle, (3.14): the dependence on the norm of the initial conditions is absent.

Ahead of the interface $x < s(t)$

$$\begin{aligned} & |\int_0^t e^{-\gamma(t-\tau)} \frac{e^{-(x-s(\tau))^2/4(t-\tau)}}{\sqrt{4\pi(t-\tau)}} v(\tau) d\tau| \\ \leq & \; V_0 \int_0^t e^{-\gamma(t-\tau)} \exp\{-\frac{(x-s(t))^2 + 2(x-s(t))(s(t)-s(\tau)) + (s(t)-s(\tau))^2}{4(t-\tau)}\} \frac{d\tau}{\sqrt{4\pi(t-\tau)}} \\ \leq & \; \frac{V_0}{\sqrt{\pi}} \exp\{-\frac{v_0|x-s(t)|}{2} - \frac{|x-s(t)|^2}{4t}\} \times \\ & \int_0^t \exp\{-\frac{(s(t)-s(\tau))^2}{4(t-\tau)} - \gamma(t-\tau)\} \frac{d\tau}{2\sqrt{(t-\tau)}} \\ \leq & \; \frac{V_0}{\sqrt{\pi}} \exp\{-\frac{v_0|x-s(t)|}{2} - \frac{|x-s(t)|^2}{4t}\} \int_0^t \exp\{(-\frac{v_0^2}{4} - \gamma)(t-\tau)\} \frac{d\tau}{2\sqrt{(t-\tau)}} \\ \leq & \; \frac{V_0}{\sqrt{v_0^2 + 4\gamma}} \exp\{-\frac{v_0|x-s(t)|}{2} - \frac{|x-s(t)|^2}{4t}\} \end{aligned}$$

To estimate the free-interface contribution to the solution $|\Psi(x,t)|$ *behind the interface* $x > s(t)$ we split the interval of integration into two subsets: $\chi_1 = \{\tau \in [0,t] : s(\tau) < (s(t)+x)/2\}$ and its complement $\chi_2 = \{\tau \in [0,t] : s(\tau) > (s(t)+x)/2\}$.

$$\int_0^t G(x,t,s(\tau),\tau) e^{-\gamma(t-\tau)} |v(\tau)| d\tau = \int_{\chi_1} + \int_{\chi_2} = I_1 + I_2,$$

For the first integral we have

$$
\begin{aligned}
I_1 &= \int\limits_{\chi_1} \frac{\exp[-(x-s(\tau))^2 \frac{1}{4(t-\tau)}]}{2\sqrt{\pi(t-\tau)}} e^{-\gamma(t-\tau)}\, |v(\tau)| d\tau \\
&\leq \frac{V_0}{2\sqrt{\pi}} \int\limits_{\chi_1} (t-\tau)^{-1/2} \exp[-(x-s(t))^2 \frac{1}{16(t-\tau)}] e^{-\gamma(t-\tau)} d\tau \\
&\leq \frac{V_0}{2\sqrt{\pi}} \int\limits_{\chi_1} (t-\tau)^{-1/2} \exp[-(x-s(t)) \frac{v_0}{8}] e^{-\gamma(t-\tau)} d\tau \\
&\leq \frac{V_0}{2\sqrt{\pi}} \exp[-(x-s(t)) \frac{v_0}{4}] \int\limits_0^{(x-s(t))/(2v_0)} \eta^{-1/2} e^{-\gamma\eta} d\eta \\
&= \frac{V_0}{2\sqrt{\gamma}} \operatorname{erf}\left(\sqrt{\gamma \frac{x-s(t)}{2v_0}}\right) \exp[-(x-s(t)) \frac{v_0}{4}] \leq \frac{V_0}{2\sqrt{\gamma}} \exp[-(x-s(t)) \frac{v_0}{4}]
\end{aligned}
$$

The following inequalities

$$
(x-s(\tau))^2 \frac{1}{(t-\tau)} \leq (\frac{x-s(t)}{2})^2 \frac{1}{(t-\tau)} \leq (\frac{x-s(t)}{2})^2 \frac{2v_0}{x-s(t)}
$$

have been used to replace the exponent in the Gaussian kernel, which gave rise to the exponential decay factor.

For the integral I_2 we obtain

$$
I_2 = \int\limits_{\chi_2} \frac{e^{-\gamma(t-\tau)}}{2\sqrt{\pi(t-\tau)}} \exp[-\frac{(x-s(\tau))^2}{4(t-\tau)}]\, |v(\tau)| d\tau
$$

$$
\leq V_0 \int\limits_{(x-s(t))/(2V_0)}^{\infty} \frac{1}{2\sqrt{\pi\eta}} e^{-\gamma\eta} d\eta = \frac{V_0}{\sqrt{\pi}} \int\limits_{\sqrt{(x-s(t))/(2V_0)}}^{\infty} \exp(-\gamma\xi^2) d\xi
$$

$$
\leq \begin{cases} \dfrac{V_0}{2\sqrt{\gamma\pi}} \exp(-\gamma(x-s(t))/(2V_0)), \text{ for } \gamma(x-s(t))/(2V_0) > 1 \\ \dfrac{V_0}{2\sqrt{\gamma}}, \text{ for } 0 \leq \gamma(x-s(t))/(2V_0) < 1 \end{cases} \tag{3.19}
$$

The final inequalties in the above estimate are based on the following elementary observations: if $a\sqrt{b} > 1$ then

$$
\int_a^{\infty} \exp(-b\eta^2) d\eta = \frac{1}{\sqrt{b}} \int_{a\sqrt{b}}^{\infty} \exp(-\eta^2) d\eta \leq \frac{1}{\sqrt{b}} \int_{a\sqrt{b}}^{\infty} \eta \exp(-b\eta^2\} d\eta = \frac{1}{2\sqrt{b}} \exp(-ba^2);
$$

on the other hand

$$\int_a^\infty \exp(-b\eta^2)d\eta \le \int_0^\infty \exp(-b\eta^2)d\eta = \frac{\sqrt{\pi}}{2\sqrt{b}}$$

Thus for $x > s(t)$ we obtain

$$|\Psi(x,t)| \le \begin{cases} \frac{V_0}{2\sqrt{\gamma}}\exp[-(x-s(t))\frac{v_0}{4}]+ \\ \frac{V_0}{2\sqrt{\gamma}}\exp(-\gamma(x-s(t))/(2V_0)), \text{ for } \gamma(x-s(t))/(2V_0) > 1 \\ \frac{V_0}{2\sqrt{\gamma}}\exp[-(x-s(t))\frac{v_0}{4}]+ \\ \frac{V_0}{2\sqrt{\gamma}} \text{ for } 0 < \gamma(x-s(t))/(2V_0) < 1 \end{cases} \tag{3.20}$$

■

Obviously the direct contribution from the initial conditions is bounded by the norm of the initial conditions:

$$e^{-\gamma t}\int_{-\infty}^{\infty} G(x,t,\xi,0)u_0(\xi)d\xi \le \frac{e^{-\gamma t}}{2\sqrt{t\pi}}||u_0||\int_{-\infty}^{\infty}\exp\{-\frac{(x-\xi)^2}{4t}\}d\xi = e^{-\gamma t}||u_0|| \tag{3.21}$$

4 Estimate for the derivative

The proof of compactness is based on a version of Arcela-Ascoli theorem and uses an estimate for the derivative of the solution. Via differentiation of the representation of the solution (2.5), the derivative for $x \neq s(t)$ is expressed as follows:

$$u_x(x,t) = -e^{-\gamma t}\int_{-\infty}^{\infty} G_\xi(x,t,\xi,0)u_0(\xi)d\xi + \int_0^t G_\xi(x,t,s(\tau),\tau)e^{-\gamma(t-\tau)}v(\tau)d\tau, \tag{4.22}$$

Lemma 4 *Let $v(t)$ be a continuous function on $[0,T]$, define the derivative of the boundary contribution as*

$$\Phi(x,t) = \frac{\partial}{\partial x}\int_0^t G(x,s(\tau),t-\tau)e^{-\gamma(t-\tau)}v(\tau)d\tau \tag{4.23}$$

Then for every $0 < t \le T$ $\quad |\Phi(x,t)| \le const$

Proof. *The estimate ahead of the front, i.e. for $x \le s(t)$*, is treated as follows. In the estimates ahead of the interface we replace $\exp(-\gamma(t-\tau))$ by 1. Consider separately two cases: $|s(t)-x| > 1$ and $|s(t)-x| \le 1$.

For the case $|s(t)-x|>1$

$$|\Phi(x,t)| = |\int_0^t \frac{x-s(\tau)}{2(t-\tau)} \frac{e^{-(x-s(\tau))^2/4(t-\tau)}}{\sqrt{4\pi(t-\tau)}} e^{-\gamma(t-\tau)} v(\tau)d\tau|$$

$$= |\int_0^t \frac{(x-s(\tau))^2}{2(t-\tau)(x-s(\tau))} e^{-(x-s(\tau))^2/8(t-\tau)} \times e^{-(x-s(\tau))^2/8(t-\tau)} \frac{v(\tau)d\tau}{\sqrt{4\pi(t-\tau)}}|$$

$$\leq |\int_0^t \frac{4/e}{s(t)-s(\tau)} \times$$

$$\exp\{-\frac{(x-s(t))^2 + 2(x-s(t))(s(t)-s(\tau)) + (s(t)-s(\tau))^2}{8(t-\tau)}\} \frac{v(\tau)d\tau}{\sqrt{\pi(t-\tau)}}|$$

$$\leq \frac{4V_0}{v_0 e\sqrt{\pi}} \int_0^t (t-\tau)^{-3/2} e^{-(x-s(t))^2/8(t-\tau)} e^{-v_0|x-s(t)|/4} e^{-v_0^2(t-\tau)/8} d\tau$$

$$\leq \frac{4V_0 e^{-v_0|x-s(t)|/4}}{e\sqrt{\pi}v_0|s(t)-x|} \int_0^t |s(t)-x|(t-\tau)^{-3/2} e^{-(x-s(t))^2/8(t-\tau)} d\tau$$

$$\leq \frac{32\sqrt{2}V_0 e^{-v_0|x-s(t)|/4}}{e\sqrt{\pi}v_0|s(t)-x|} \int_0^\infty e^{-\eta^2} d\eta \leq \frac{16\sqrt{2}V_0}{ev_0} \frac{e^{-v_0|x-s(t)|/4}}{|s(t)-x|} \tag{4.24}$$

In the last estimate we used the following simple observations: $\xi e^{-\xi} \leq 1/e$, for $\xi = \frac{(x-s(\tau))^2}{8(t-\tau)} > 0$, $|s(\tau)-x| > |s(t)-x|$, $|s(\tau)-x| > |s(t)-s(\tau)| > v_0|t-\tau|$ and substitution $\eta = |s(t)-x|(t-\tau)^{-1/2}/\sqrt{8}$ to obtain the error function integral.

For the less involved case $|s(t)-x| \leq 1$ we split the integral into two parts

$$|\Phi(x,t)| = |\int_0^t \frac{x-s(\tau)}{2(t-\tau)} \frac{e^{-(x-s(\tau))^2/4(t-\tau)}}{\sqrt{4\pi(t-\tau)}} v(\tau)d\tau|$$

$$\leq |\int_0^t \frac{|x-s(t)| + |s(t)-s(\tau)|}{2(t-\tau)} \frac{e^{-(x-s(\tau))^2/4(t-\tau)}}{\sqrt{4\pi(t-\tau)}} v(\tau)d\tau|$$

$$\leq \frac{V_0}{\sqrt{\pi}} \int_0^t \frac{|s(t)-x|(t-\tau)^{-3/2}}{4} e^{-(x-s(t))^2/4(t-\tau)} d\tau + \frac{V_0^2}{4\sqrt{\pi}} \int_0^t \frac{e^{-(s(t)-s(\tau))^2/4(t-\tau)}}{\sqrt{(t-\tau)}} d\tau$$

$$\leq \frac{V_0}{\sqrt{\pi}} \int_0^\infty e^{-\eta^2} d\eta + \frac{V_0^2}{4\sqrt{\pi}} \int_0^t \frac{e^{-v_0^2(t-\tau)/4}}{\sqrt{(t-\tau)}} d\tau$$

$$\leq \frac{V_0}{2} + \frac{V_0^2}{v_0\sqrt{\pi}} \int_0^\infty e^{-\xi^2} d\xi = \frac{V_0}{2}(1 + \frac{V_0}{v_0}) \tag{4.25}$$

where $\eta = (x-s(t))(t-\tau)^{-1/2}/2$ and $\xi = v_0\sqrt{(t-\tau)}/2$.

Thus, collecting estimates in (4.24)-(4.25) we observe that the derivative ahead of the interface $x < s(t)$ decays exponentially

$$|\Phi(x,t)| \leq \begin{cases} \dfrac{16\sqrt{2}}{ev_0} e^{-v_0|x-s(t)|/4} V_0, \ x < s(t) - 1 \\ \dfrac{V_0}{2}(1 + \dfrac{V_0}{v_0}), \ s(t) - 1 \leq x \leq s(t) \end{cases} \tag{4.26}$$

The part of the *estimate concerning the derivative behind the interface* $x > s(t)$ causes some difficulties due to the fact that x can be close or even equal to $s(\tau)$; it is treated as follows. For our purposes it suffices to prove the estimate for t starting from a certain $t > 0$. Assume for convenience that $t > 1$. For the second integral in (4.22) we split the interval of integration into two subsets: $\chi_1 = \{\tau \in [0,t] : |s(\tau) - x| \geq |s(t) - x|/2\}$ and its compliment $\chi_2 = [0,t] \setminus \chi_1$. Note again that $s(t)$ is a monotone function. We have

$$\left| \int_0^t G_\xi(x,t,s(\tau),\tau) e^{-\gamma(t-\tau)} v(\tau) d\tau \right| \leq \int_0^t |G_\xi(x,t,s(\tau),\tau) e^{-\gamma(t-\tau)}| \times |v(\tau)| d\tau \tag{4.27}$$

$$= \int\limits_{\chi_1} + \int\limits_{\chi_2} = I_1 + I_2, \tag{4.28}$$

For I_1 we use two subsets of χ_1: $\chi_1 = \chi_{11} \cup \chi_{12}$ where $x > s(\tau)$ for χ_{11} and $x < s(\tau)$ for χ_{12}. For the integrals we get respectively

$$\begin{aligned} I_{11} &= \int\limits_{\chi_{11}} \frac{|x - s(\tau)|}{2(t-\tau)} \times \frac{\exp[-\dfrac{(x-s(\tau))^2}{4(t-\tau)}]}{2\sqrt{\pi(t-\tau)}} e^{-\gamma(t-\tau)} \times |v(\tau)| d\tau \\ &\leq \frac{2V_0}{\sqrt{\pi}} \int\limits_0^\infty |x - s(t)|(t-\tau)^{-3/2} \exp[-(x-s(t))^2 \frac{1}{16(t-\tau)}] d\tau \\ &\leq \frac{2V_0}{\sqrt{\pi}} \int\limits_0^\infty e^{-\xi^2} d\xi = V_0 \end{aligned} \tag{4.29}$$

(note that on χ_{11} $|x-s(t)|/2 < |x-s(\tau)| < |x-s(t)|$). In the above integral we have made a substitution $|x-s(t)|(t-\tau)^{-1/2}/4 = \xi$. For the second part

$$
\begin{aligned}
I_{12} &= \int\limits_{\chi_{12}} \frac{|x-s(\tau)|}{2(t-\tau)} \times \frac{\exp[-\dfrac{(x-s(\tau))^2}{4(t-\tau)}]}{2\sqrt{\pi(t-\tau)}} e^{-\gamma(t-\tau)} \times |v(\tau)| d\tau \\
&\leq \int\limits_{\chi_{12}} \frac{|s(t)-s(\tau)|}{2(t-\tau)} \times \frac{\exp[-\dfrac{(x-s(\tau))^2}{4(t-\tau)}]}{2\sqrt{\pi(t-\tau)}} e^{-\gamma(t-\tau)} \times |v(\tau)| d\tau \\
&\leq \frac{V_0^2}{4} \int\limits_0^t \frac{e^{-\gamma(t-\tau)}}{\sqrt{\pi(t-\tau)}} d\tau \leq \frac{V_0^2}{4\sqrt{\pi\gamma}} \int\limits_0^\infty \frac{e^{-\tau}}{\sqrt{\tau}} d\tau = \frac{V_0^2}{4\sqrt{\gamma}}
\end{aligned}
\tag{4.30}
$$

We remark that a time independent estimate for the above integral is also valid.

For I_2 we shall replace a function of the type xe^{-x^2} by its maximum $1/\sqrt{2e}$

$$
\begin{aligned}
I_2 &= \int\limits_{\chi_2} \frac{|x-s(\tau)|}{2(t-\tau)} \times \frac{\exp[-\dfrac{(x-s(\tau))^2}{4(t-\tau)}]}{2\sqrt{\pi(t-\tau)}} e^{-\gamma(t-\tau)} \times |v(\tau)| d\tau \\
&\leq V_0 \int\limits_{\chi_2} \frac{|x-s(\tau)|}{2\sqrt{(t-\tau)}} \times \exp[-\frac{(x-s(\tau))^2}{4(t-\tau)}] \times \frac{1}{2\sqrt{\pi}(t-\tau)} d\tau \\
&\leq \frac{1}{\sqrt{8\pi e}} V_0 \int\limits_{\chi_2} \frac{d\tau}{(t-\tau)} \leq \frac{1}{\sqrt{8\pi e}} V_0^2 \int\limits_{\chi_2} \frac{d\tau}{|s(t)-x|/2} \leq \frac{V_0^2}{v_0\sqrt{2\pi e}}
\end{aligned}
\tag{4.31}
$$

We have also replaced $(t-\tau)$ in the denominator by its minimum $|s(t)-x|/2\,\|v\|$ on $\chi_2$and observe that $meas(\chi_2) \leq |s(t)-x|/v_0$.

By collecting the estimates in (4.29)-(4.31) we obtain a uniform bound for the derivative behind the interface $x > s(t)$,

$$
|\Phi(x,t)| \leq V_0 + \frac{V_0^2}{4\sqrt{\gamma}} + \frac{V_0^2}{v_0\sqrt{2\pi e}} \tag{4.32}
$$

This concludes the proof of the lemma. ■

We also note that the first term in (4.22) can be easily estimated,

$$
\begin{aligned}
\left|\int_{-\infty}^\infty G_\xi(x,t,\xi,0) u_0(\xi) e^{-\gamma t} d\xi\right| &\leq e^{-\gamma t} \int_{-\infty}^\infty \frac{|x-\xi|}{2t} \times \frac{\exp[-\dfrac{(x-\xi)^2}{4t}]}{2\sqrt{\pi t}} |u_0(\xi)| d\xi \\
\leq ||u_0|| \frac{e^{-\gamma t}}{\sqrt{\pi t}} \int_{-\infty}^\infty \frac{|x-\xi|}{2\sqrt{t}} &\times \exp[-\frac{(x-\xi)^2}{4t}] \times \frac{d\xi}{2\sqrt{t}} \leq ||u_0|| \frac{e^{-\gamma t}}{\sqrt{\pi t}}
\end{aligned}
$$

since the integral on the last line is equal to $2\int_0^\infty \eta \exp(-\eta^2) d\eta = 1$, with $\eta = |x-\xi|/2\sqrt{t}$. Thus we get the following

Corollary 5 *For any $t \geq t_0$, $t_0 > 0$, the derivative of the solution is uniformly bounded:*

$$|u_x(x,t)| = ||u_0|| \frac{e^{-\gamma t}}{\sqrt{\pi t}} + C \tag{4.33}$$

We reiterate that the proof of compactness in the next section is based on a version of Arcela-Ascoli theorem and uses the estimate for the derivative of the free-interface contribution, $|\Phi(x,t)| \leq const$. Thus the estimates of this section are crucial for the compactness result.

5 Absorbing set and attractor

In this section we use the estimates obtained above to establish existence of a bounded absorbing set and of the attractor which is compact in the space of continuous functions. It can be easily verified that all the estimates and analytical properties of the solutions can be obtained without the heat losses. On the other hand the problem with the heat losses exhibits uniform exponential decay in time of the contribution from the initial data which is utilized in the proof of compactness of the attractor.

The integral representation (2.5) describes the evolution of the initial temperature distribution u_0: $u(t) = T(t)u_0$. We think of the evolution as taking place for the functions on $(-\infty, \infty)$ in the moving coordinate system attached to the free boundary $x' = x - s(t)$. Note that all the results in Sec. 3-4 are in tems of x'.

It is convenient to split the semigroup operator T into two parts: the contribution of the free boundary

$$T_1(t)u_0(x') = -\int_0^t e^{-\gamma(t-\tau)} G(x' + s(t), t, s(\tau), \tau) v(\tau) d\tau \tag{5.1}$$

and that of the initial data

$$T_2(t)u_0(x') = e^{-\gamma t} \int_{-\infty}^{\infty} G(x' + s(t), t, \xi, 0) u_0(\xi) d\xi \tag{5.2}$$

We rephrase the esimates in (3.21) and (3.16) as the following result that establishes existence of an absorbing set for the evolution.

Proposition 6 *(i) The semigroup T_2 is uniformly exponentially contracting in C:*

$$\sup_{u^0 \in X} ||T_2(t)u^0|| \leq \exp(-\gamma t) N$$

for any ball

$$X = \{u \in C; \quad ||u|| \leq N\}$$

(ii) For any $\varepsilon > 0$, the ball $B_{abs} := \{u \in C : \quad |u| \leq V_0/(2\sqrt{\gamma}) + \varepsilon\}$ is an absorbing set for all bounded subsets of C for the semigroup T. Here the radius of the absorbing ball reflects the contribution of the free interface alone.

Next we prove that the boundary contribution to the evolution, i.e. the operators $T_1(t)$ are *uniformly compact*. Namely, the following proposition holds:

Proposition 7 *For any $t_0 > 0$ the orbit of the ball $O(X, t_0) = \cup_{t \geq t_0} T_1(t)X$ is relatively compact in C.*

Proof. For the version of Arzela-Ascoli theorem appropriate for C it is sufficient to have uniform boundedness for the derivative and uniform decay of the family of functions as $|x'| \to \infty$. From Lemma3 we see that for the initial data in a ball, the contribution from the interface exhibits a spatial decay uniformly with respect to time. On the other hand, the estimate (**??**) demonstrate that the spatial derivative is uniformly bounded.

Now it is a simple matter to construct a finite ε-net for $O(X, t_0)$. First we choose a finite interval $-L \leq x' \leq L$, beyond which the functions of the family are smaller than ε, it is possible to accomplish because of the uniform in time spatial decay. In view of the uniform bound on the derivative, the functional family is equicontinuous. Therefore the restricion of $O(X, t_0)$ on to $[-L, L]$ is compact by the regular Arzela-Ascoli theorem. By extending the elements of the ε-net from $[-L, L]$ to the whole line by zero we obtain an ε-net in $O(X, t_0)$. ■

The properties of the evolution operator $T(t)$ described in the above propositions allow us to apply the abstract general result (see, for example, [23, Chap. 1]) that in our situation can be stated as follows:

Theorem 8 *The ω-limit set $\mathcal{A}$ of the absorbing set B_a is a global exponential compact attractor for the metric space C; $\mathcal{A}$ is the maximal attractor in C and it is connected.*

6 Numerical dimension of attractor

Having proved compactness one is naturally curious as to how "large" is the attractor in terms of some appropriate measure? For the one-phase problem we have been able to prove that the Hausdorff dimension of the attractor is finite [11]. However, due to the additional temperature field behind the propagating interface (in the product phase), methods of the papers dealing with the one-phase problem are not directly applicable to the two-phase problem. Currently we are not able to overcome these, we believe, purely technical difficulties, although we have little doubt that the dimension is finite for the two-phase case as well.

The question arises also, whether the presence of the temperature field behind the front affects the "size" of the attractor in comparison with the one-phase case (see [12]). We provide an answer to this question by computing the correlational dimension of the attractors generated via direct numerical simulation of the problem.

While the Hausdorff dimension is convenient for analytical estimates, it is highly non-trivial to compute and requires too much storage and CPU time. More convenient computationally is the *correlation dimension.* Although in general $d_{corr} \leq d_{Hausdorff}$, they are usually very close. We follow the now standard procedure for computation of the correlation dimension [16]. Namely, consider the set $\{U_i,\ i = 1, ...N\}$ of points on the attractor $U_i = U(T + i\tau)$, where $T \gg 1$. We consider a discreet approximation of the solution in the space $\mathbb{R}^k$ by sampling the solution at k points $U_i = (u(x_1, T + i\tau), ..., u(x_k, T + i\tau))$. We measure the spatial correlation between the points on the discreet approximation of the attractor with the correlation integral

$$C(l) = \lim_{N\to\infty} \frac{1}{N^2}\{\text{number of pairs with the distance } \rho(U_i, U_j) < l\}$$

If for small l, $C(l)$ scales as l^ν then the correlation exponent ν can be taken as the correlation dimension of the attractor d_{corr}. For practical calculations the frequency of sampling τ, the number k of points in space where the solution is sampled at each time, and the number of samples N are determined empirically. Similarly, for the low sample dimension k a better approximation for d_{corr} may be obtained if the Euclidean distance ρ is modified by inclusion of a weight.

To obtain a numerical approximation of the attractors we solve the initial value problem (2.1)-(2.4) for sufficiently large time until the asymptotic regime is attained. Obviously the dimension of the attractor should not depend on the choice of initial data, which was confirmed by direct numerical simulations. Problem (2.1)-(2.4) was solved in the frame attached to the free boundary on a finite interval $[-L, L]$ with the Dirichlet conditions $w(-L, t) = 0$ simulating the decay of the solution at $-\infty$, and $\partial w(L, t)/\partial x = 0$ corresponding to the stabilization of the temperature in the product phase. According to our observations the results are practically insensitive to the increase in the interval length after $L \sim 30$ (see [7] for the details of the numerical algorithm). We remark that in contrast with the one-phase case where $L \sim 10$ was sufficient, one needs a rather large spatial domain to obtain consistent numerical results.

To represent different dynamical regimes we use the Arrhenius kinetics ,

$$V = g(u) := -\exp[\alpha \frac{u - 1}{\sigma + (1 - \sigma)u}], \tag{6.3}$$

where (in the context of combustion) α is proportional to the activation energy (Zeldovich number), and σ is the temperature ratio of the fresh mixture and the product, see e.g. [7].

Thus, the attractor is represented as a set in $\mathbb{R}^k$, where k is the number of sampling points of temperature profiles. We choose time snapshots of the solution for every 0.08 in the interval of the asymptotic regime ($200 < t < 1800$) and consider them as a discrete approximation of the attractor in $\mathbb{R}^k$. The correlation dimension for this discrete set is evaluated as explained above. As a control experiment we selected a periodic asymptotic regime, $\alpha = 4.5$. It is immediately confirmed that $d_{corr} \approx 1$ as one should expect.

In contrast, for $\alpha = 5$, $\sigma = 0.05$ the regime is chaotic as is illustrated in Fig. 1 that presents a series of snapshots of spatial temperature profiles. One can see from the log-log

Figure 1: Time history $0 < t < 4000$ for chaotic dynamics $u(x,t)$ vs. x, t.

graph of the correlation integral (Fig. 2) that in this case $d_{corr} \approx 2$. From our observations on a variety of regimes it appears that the dimension cannot be much higher than 2.

7 Concluding remarks

The compactness result has been proved here in the presence of heat losses for any nonzero heat loss. Although we chose to operate in spaces of continuous uniformly bounded functions on the infinite interval, we are convinced that compactness can be established even for zero heat loss if spaces with weaker topology are used, for instance in the space of continuous functions bounded on each finite interval.

Results of this paper have been proved for the kinetic function satisfying the bounds in (**??**). These bounds are quite physical and cover a wide range of important applications. Nonetheless, our numerical experimentation with different types of kinetic functions, including unbounded ones demonstrate that the asymptotic dynamics are insensitive to the

Figure 2: Correlation integral for 7-, 8- and 9-point samples.

behavior of the kinetic function for large temperatures. On the other hand, our results from [6] provide global existence and uniform boundedness of solutions for a wider class of kinetic functions, namely for sublinear kinetics. Therefore we strongly believe that the principal result of this paper holds for this case as well.

It is interesting to compare the proof of the compactness above to that for the one-phase problem [10]. Although the estimates in the two-phase case are more involved due to the presence of the temperature field behind the propagating interface, once they are obtained, the representation of the evolution semigroup is more transparent than in the one-phase case.

Also, it is rather remarkable that the numerical estimates for the correlation dimension of the attractor above and for the one-phase case (see [12]) yield roughly the same value. Indeed, such an outcome is rather unexpected because the two-phase problem seems to

possess more ”degrees of freedom” than its one-phase counterpart.

Finally, for the one-phase problem we have been able to prove that the Hausdorff dimension of the attractor is finite [11]. Currently we are not able to overcome certain difficulties that we believe are of purely technical nature but it appears safe to conjecture that the dimension of the attractor is finite for the two-phase problem as well.

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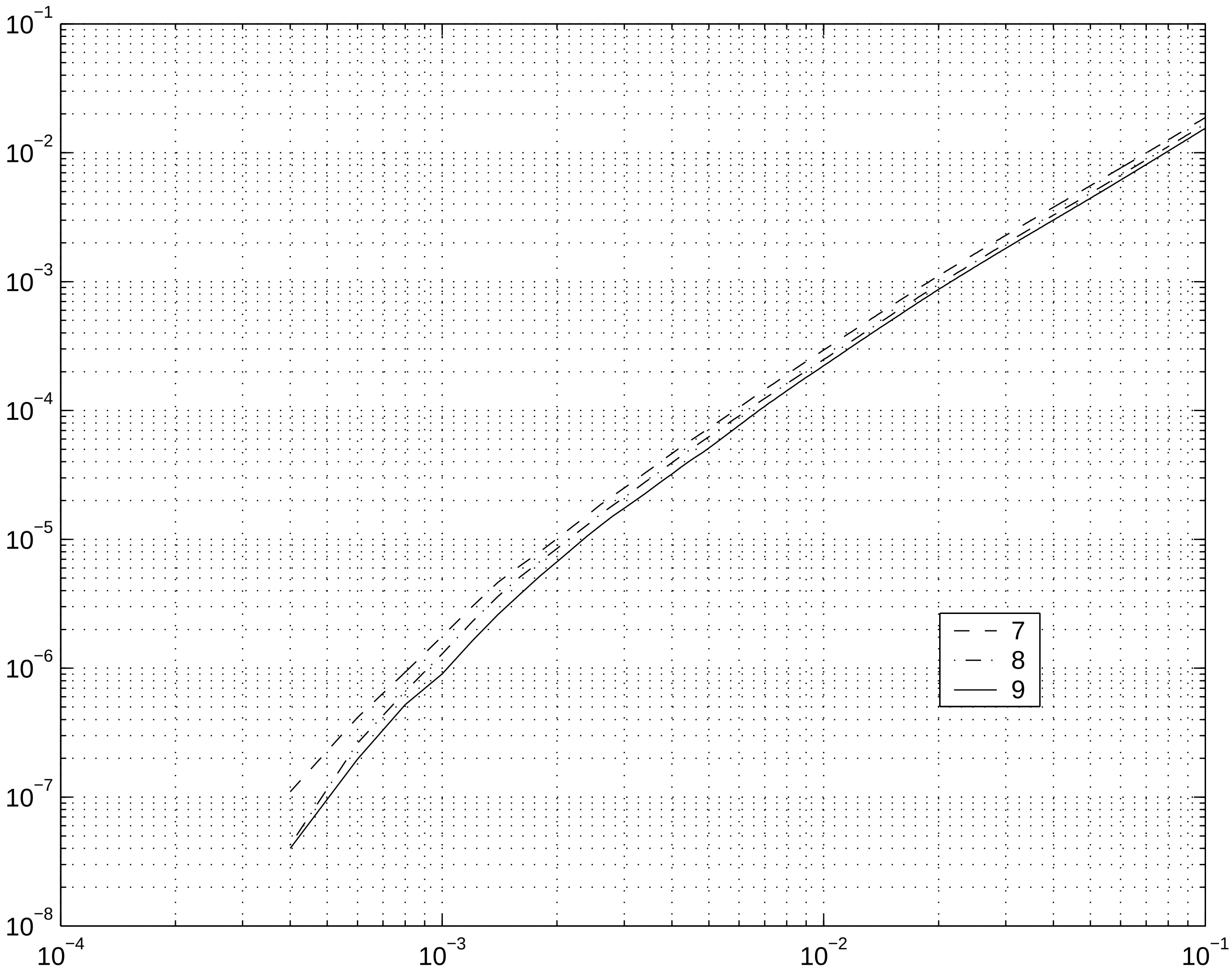

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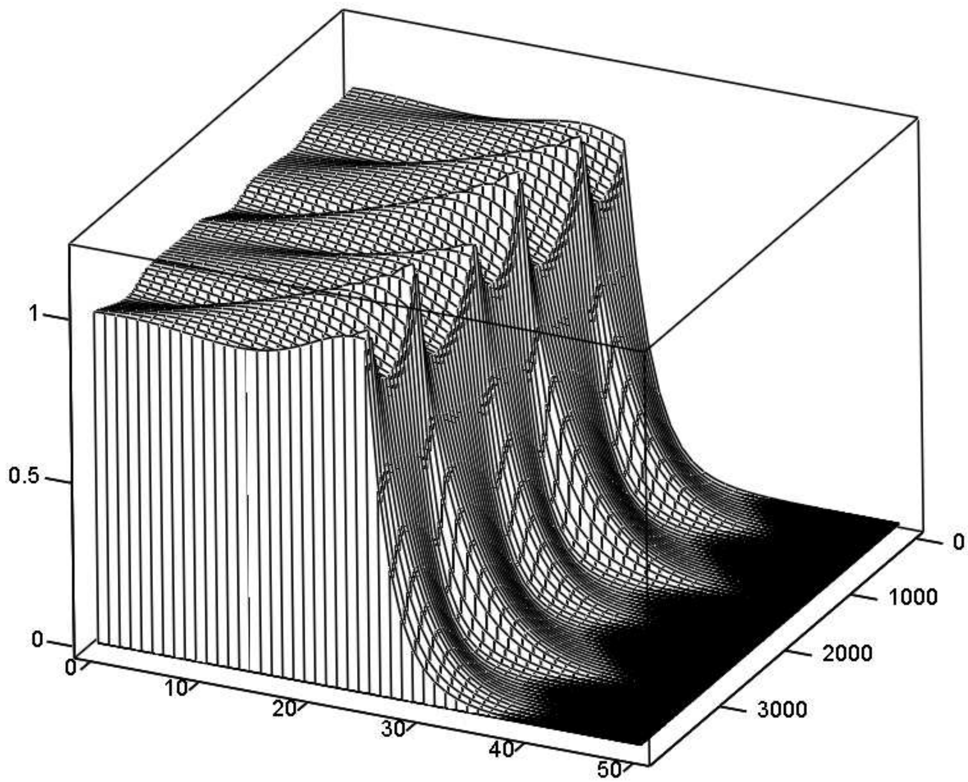

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